Neutronics Analysis of Molten Uranium Breeder Reactor with a Code-to-Code Verification

Christian Pochron¹, Zeyun Wu¹, Neal Mann², and Mihai (Mike) Pop³

¹Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University, Richmond, VA ²Neal Mann and Associates, Washington DC ³Areva College of Experts (Retired), Alexandria, VA pochronc@vcu.edu; zwu@vcu.edu; neal@nealmannnuclear.com; mihaigm@aol.com

INTRODUCTION

The Molten Uranium Breeder Reactor (MUBR) is a conceptual reactor design that can solve one of the largest issues for the nuclear power industry: nuclear waste. The MUBR is a breed and burn reactor that can utilize Low Enriched Uranium (LEU) fuel or a mixture of Used Nuclear Fuel (UNF) and LEU fuel. The breed and burn capabilities allow the MUBR to operate with the initial fuel for 50+ years with no manipulation of the fuel during that period of time [1]. Thus, allowing UNF to be utilized to produce power instead of sitting in a storage cask. A majority of the fissions occur in the fast energy range. U-238 will direct fission due to fast neutrons (~20%) or absorb a neutron and β -decay to Pu-239 which is then fissile (~80%) [1].

The MUBR design utilizes features found in CANDU reactors and molten salt reactors [2]. The MUBR design uses heavy water as a moderator and reflector to reduce neutron leakage and increase the conversion ratio [1]. The MUBR design will also utilize a gas cover to capture any fission products that will evaporate. The MUBR operates with the molten fuel between 1200°C and 1400°C [2]. Due to such a high operating temperature, many of the fission products will evaporate. Due to this the gas cover will allow the evaporated fission products to be removed from the fuel. The unique feature of the MUBR design influenced the nuclear simulation software used to analyze the idea.

METHOD

Computational Tools

The analysis of the MUBR will be performed with two well-known neutronics analysis software: MCNP and SCALE. Therefore a code-to-code verification working philosophy is implemented all through the neutronics analysis procedure. MCNP is a Monte Carlo method-based software developed by Los Alamos National Laboratory [3]. SCALE is a nuclear modeling and simulation tool package developed by Oak Ridge National Laboratory [4]. Both MCNP and SCALE can be used for critical safety, reactor physics, depletion analysis, and to investigate the sensitivity of the MUBR design. MCNP offered the ability to create the complex structure of the MUBR design. SCALE was selected due to a feature that can filter/remove materials and store them elsewhere. This can also be accomplished in MCNP but it would be more difficult to implement. Each software will run the same tests with the same input parameters. Comparing the results obtained from the tests will provide valuable information for further studies of the reactor design.

The MUBR design was originally created in MCNP and is now being built in SCALE. The burnup simulations based on MCNP6 on a MUBR configuration confirmed the primary neutronic feasibility of the reactor [1]. SCALE will be utilized to confirm these results and implement new features for more accurate analysis.

A special utility tool named MCNP6gen was developed to facilitate the creation of the MUBR input for SCALE and/or MCNP [2]. MCNP6gen is a useful tool to quickly change and develop the input for both software. MCNP6gen can run different tests while automatically changing a single dimension of the input for each iteration. This feature was useful in finding the optimal diameter of the fuel tubes. This tool will not be useful if the inputs for MCNP and SCALE are not identical and generate the same reactor design. The inputs must create the exact same reactor to accurately compare the results provided from MCNP and SCALE.

Computational Models

A nearly complete MUBR core is currently created in MCNP. To reduce the run time and complexity of the comparison between the MCNP and SCALE codes, a more simplified version of the MUBR core is modeled instead by both codes. This core allows for easy changes and less computational cost. The core we focused on in this study contains a 37-pin hexagonal fuel tube array as shown in Figure 1. The fuel tubes are 30 centimeters in diameter and have silicon-carbide cladding. Through these tubes, will flow the molten uranium. The 1475 K molten uranium is 0.96% ²³⁵U and 99.04% ²³⁸U by weight. Figure 2 offers an axial view of the core. Figure 2 shows the separation between the heavy water moderator and the helium gas. The heavy water steam will moderate the neutrons in the lower half of the core. Once the fuel enters the helium region, fissions will cease due to the inert gas. Both Figure 1 and Figure 2 are rendered by the SCALE models. The MCNP model has a very similar views of the core. This design has a heavy water steam moderator and half of the upper portion of the core is filled with helium. The core has the same major characteristics as the complete MUBR design.



Figure 1. Axial Core View of the MUBR Core in SCALE.



Figure 2. Side View of the MUBR Core in SCALE.

RESULTS

MCNP6gen generated a series of inputs for MCNP and SCALE. These inputs represented various versions (refer to as Version 1 - 4 thereafter) of the simplified MUBR cores. These versions were generated with varied material properties to optimize the reactor performance. Each version was tested and compared to determine any differences between them. After each run, revisions were made to MCNP6gen to create more comparable inputs for MCNP and SCALE.

Version 1 had shown the largest difference of 2025 pcm (per cent mille) in keff. This is because although MCNP6gen generated the same geometries for SCALE and MCNP, the materials differed drastically. The SCALE input had the wrong materials for the fuel tubes, helium gas, and had different compositions for the heavy water steam. MCNP6gen was corrected to gain a better match to the materials in the MCNP input for the core. With these changes, Version 2 results were generated, in which the material in MCNP was defined in atom fraction, whereas in SCALE it is specified by atomic number density. MCNP6gen did not properly convert between atom fraction and atomic number density, and thus resulted with a large difference in the isotopic composition of the materials. Version 2 resulted

with a difference of 261 pcm in keff. Version 3 corrected the isotopic compositions of the materials, and achieved a difference of 62 pcm in keff.

Although the difference in keff was shown satisfactory in Version 3, there is some inconsistencies noticed on the use of nuclear data energy structure in the two codes. The SCALE utilized ENDF/B-VII.1 252-group multigroup cross section data [4], whereas MCNP uses ENDF/B-V continuous energy cross section data. Furthermore, SCALE automatically applies the thermal scattering law to the moderator, whereas the thermal scattering function must be additionally attached to the moderator specification in MCNP. After applying the continuous energy cross section data and the thermal scattering law for moderators to both codes, Version 4 results were generated and reached a difference of 98 pcm in keff between the SCALE and MCNP, which is acceptable for the simplified MUBR code-to-code verification procedure with the consideration of the 1σ statistical errors (see Table I).

Table I. MCNP-SCALE keff Comparison in Version 4

MCNP	SCALE	∆keff
1.00053 ± 0.00014	0.99955 ± 0.00017	0.00098

CONCLUSIONS

The code-to-code verification procedure was a necessary step to ensure that the MCNP and SCALE results were comparable for the new reactor analysis. Several versions of the special utility tool MCNP6gen were fine-tuned to ensure the material composition, structural configuration, and nuclear data were all identical. The final version of MCNP6gen created MCNP and SCALE results within 98 pcm which is deemed acceptable for the simplified MUBR design code-to-code verification. For the future work, the simplified MUBR core will continue to be used and adjusted to add more features to the MCNP and SCALE inputs. The right next step in the process is to enable the fission product removal capabilities in SCALE. Implementing these features will improve the modeling capabilities for the MUBR design.

REFERENCES

- 1. N. L. MANN and M. G. POP, "The Molten Uranium Thermal Breeder Reactor (MUTBR): A consumer of UNF," *Trans. Am. Nucl. Soc.*, **125**, 2021.
- N. L. MANN and M. G. POP, "VCU analysis discussion for the Molten Uranium Breeder Reactor (MUBR)," Neal Mann and Associates, August 22, 2022.
- J. A. KULESZA, et al., "MCNP® Code Version 6.3.0 Theory & User Manual," LANL Tech. Rep. LA-UR-22-30006, Rev. 1. Los Alamos, NM, September 2022.
- W. A. WIESELQUIST, R. A. LEFEBVRE, M. A. JESSEE. "SCALE Code System," Oak Ridge National Laboratory, April 2020.